1-Octadecanol 112-92-5 | DTXSID8026935

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Model	Data

Weighted KNN model

5-fold CV (75	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 333 °C

Global applicability domain: Inside

Local applicability domain index: 5.37e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

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Heptadecan-1-ol Measured: 333 Predicted: 331 Image not found

1-Eicosanol Measured: 372 Predicted: 362 Image not found

1-Hexadecanol Measured: 334 Predicted: 324

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1-Tetradecanol Measured: 289 Predicted: 291